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To meet the requirements set forth for the Armys Petroleum Test Kit (PTK), The Army has developed a near-infrared spectrometer, under the Small Business Innovative Research program, which utilizes chemometrics to predict various physical properties of a fuel sample. This paper was written in April of 2004 and reflects the status of the program to that date.

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U.S. Army Tank Automotive Research Development and Engineering Center

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Near-Infrared Spectroscopy and Chemometrics Instrumentation and Methodology for Field Evaluation of Diesel and Aviation Fuels by the U.S. Army

Joel Schmitigal
Force Projection Technology

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1. Introduction

To meet the requirements set forth for the Army's Petroleum Test Kit (PTK), The Army has developed a near-infrared spectrometer, under the Small Business Innovative Research program, which utilizes chemometrics to predict various physical properties of a fuel sample. This paper was written in April of 2004 and reflects the status of the program to that date.

1.1. Principles of Near-Infrared Spectroscopy (NIR)

Near infrared spectroscopy became an accepted analytical chemistry technique in the early 1960's due to work performed by the US Department of Agriculture's Karl Norris (1). NIR spectroscopy is method used in analytical chemistry that measures the absorption of electromagnetic radiation by molecular bonds causing the vibration of these bonds. These molecular vibrations fall into two basic categories: stretching and bending. Stretching vibrations involve the continuous change of the distance between the two atoms involved in the bond while bending vibrations are characterized by the change of angle between two bonds.

The near infrared range of the electromagnetic spectrum is located between the mid-infrared and visible regions, which ranges in wavelengths from 2500 nanometers down to 700 nanometers. The absorption bands that are found in the NIR region result from overtone and combination vibrations of the molecules being investigated. Overtone bands occur at approximate multiples of the frequency of the fundamental vibration that they shadow and exist at weaker intensities (2). Combination bands occur with the coupling of multiple fundamental bands and are seen at an additive or subtractive frequency. Due to the fundamental vibration frequencies most often occurring within the mid-infrared region we find the near-infrared region to be made up of overtone and combination bands.

The origins of the absorption bands come from the absorption of radiation by the molecular bond under study causing it to vibrate. When the frequency of radiation from the source matches the frequency potential of the vibrating molecules bond there is a transfer of energy to the molecule. The transfer of energy into any one bond is not continuous but happens in defined amounts of energy termed quanta; quantities of quanta are maintained in the term of vibrational quantum number. Energy absorption between the ground state energy level and the first transition level is termed a fundamental, this transition results in peaks most commonly associated with the mid-infrared region.

Transitions from the ground to the second or third energy levels and higher are termed first, second and up overtones. The frequencies of overtones approximately correspond to twice, three times and up respectively of the frequency for the fundamental transition. The more a bond varies from harmonicity the more intense is its resulting overtone band. This is why the most intense overtone bands result from bonds between hydrogen to oxygen, nitrogen, and carbon.

The third type of band that can occur in vibrational spectrometry is appearance of combination bands. Combination bands result when a photon causes two or more vibrational modes at the

same time. The interaction of the simultaneous vibrations gives rise to a band with a frequency equal to the sum or difference of the combining fundamental frequencies.

2.   Chemometrics and use in Near Infrared Spectroscopy

The term chemometrics was coined in the early 1970's by Swedish scientist Svante Wold (3). Chemometrics utilizes mathematical modeling to provide a correlation between experimental values (the NIR spectrum) and known concentrations or physical properties. Due to the near-infrared region being composed of overtone and combination bands the complexity of its interpretation has greatly popularized the use of chemometrics by chemists.

The use of chemometrics in analytical spectroscopy employs the use of multivariable data analysis, which associates multiple variables of the NIR spectrum simultaneously to known parameters of the sample. Multivariable analysis evaluates differences in a samples spectrum to given known values, concentration of analyte or physical property, to provide a correlation between the chemical structure and the known value. By developing a model that encompasses the range of expected known values we are able to create a program that can correlate the spectral output of the NIR instrument to the analyte concentration or physical property of the sample.

The use of chemometrics has found great popularity in providing a correlation between the near infrared spectrum and the physical properties of fuels. To utilize this indirect method of predicting a physical property of the fuel, a relationship must exist in the chemical structure of the sample and the property being measured. For example when determining cetane value a high amount of aromatic and aliphatic branching in the fuel will lower the cetane value, while an increase in straight chain molecules will increase the cetane value. The use of near infrared spectroscopy in not a direct measurement technique of the fuels physical property but is a correlative measurement, the accuracy of your results are entirely dependant on the quality of your correlation models.

2.1.   Application of Near-Infrared Spectroscopy to the Determination of Fuel Type

The initial use of near infrared spectroscopy in the petroleum industry was for the monitoring of octane content of gasoline during inline blending operations (4). Since the early 1990's when these process monitoring spectrometers first appeared additional models have been developed and NIR spectrometers can be found in many facets of the petroleum refinery process stream including diesel and fuel oil blending (4). Several articles have been published describing NIR and chemometrics for predicting the properties of petroleum fuels (4-15).

In the mid 1990's the US Army funded a near infrared spectroscopy research project at Southwest Research Institute (5). In this project researchers wrote calibration models for 17 fuel properties, using NIR spectrometers from three different manufacturers (5). A validation set was then run and compared to the property values reported through traditional laboratory analysis. Properties that gave a squared correlation coefficient, R^2, of .70 or greater were determined to be

successful and will be open for additional analytical consideration in development of NIR predictive models for the PTK. These properties include: API gravity, density, cloud point, freeze point, viscosity at 40 °C, boiling point at 50% distilled, cetane index, percent hydrogen, carbon/hydrogen, heat of combustion, and total aromatics. Flashpoint was also determined to be addressed in future studies due to the abundance of available data.

For the NIR spectrometer being developed for the Petroleum Test Kit this list was narrowed down to differing properties for Diesel No. 2, Diesel No. 1, JP-8, Jet-A, Jet-A1, and JP-5 based on the normal B-2 test requirements from MIL-STD-3004 (6). Due to differing properties in fuel types it is strongly desired to be able to first isolate what type of fuel a sample is and then further determine the quality of the sample. Samples can be categorized into one of three quality levels, or specification ratings. *On-spec* - fuels that meet all specifications for purchase according to MIL-STD-3004. *Off-spec* - consists of fuels that are considered acceptable for inter-service transfer according to MIL-HB-3004. And *out-of-spec* - which are fuels that fall out of acceptable limits and can not be utilized. Tables a thru d in appendix A contain the properties that the Army feels it can successfully model using NIR technology and the specification limits for each fuel and corresponding property.

3. Instrumentation

The near-infrared spectrometer that has been selected for use in the PTK is the Eliminator Near-infrared Spectrometer developed by Micron Instruments under a Small Business Innovative Research (SBIR) contract from the Army. The instrument is compact, light weight, rugged, contains no moving parts, can run off over a variety of power sources including battery. The instrument's source is a feedback stabilized high intensity tungsten halide lamp with peak intensity of 1300nm. For sampling the instrument utilizes a rugged fiber optic probe with a 10mm sample cell. The instrument employs a volume holographic transmission grating as its monochromator, and a 512 pixel InGaAs one dimensional array detector operated with a 4 millisecond shutter speed.

4. Experimental Procedure

Fuel samples were collected globally with the assistance of the Defense Energy Support Center (DESC), the Army Petroleum Center (APC), stationed and deployed Army troops, and petroleum manufacturers. Every sample was subjected to B-2 testing to determine its specification rating, additional tests where performed in instances where additional properties were determined to be advantageous when utilizing the NIR instrument.

4.1. Data Pre-treatment

Even the most novice of observers will notice the presence of spectral baseline shifting from background noise due to the bending of the optic when analyzing fuel samples with the fiber optic sampling probe. The first step in analyzing the NIR data obtained for the fuel samples is to eliminate this baseline offset. Depending on the desired effect this can be done in a multitude of ways. The two methods that have found to provide the most favorable results are taking derivatives of the spectral data and the standard normal variate method (SNV).

Taking the derivative of the NIR spectral data helps to remove background noise in spectroscopic samples. As a result of the NIR spectra being composed of individual points and not a continuous function a true derivative can not be taken for each sample, therefore the derivative is computed using the Savitzky-Golay method. The Savitzky-Golay method works by fitting a polynomial to the data around each data point within a localized spectral segment (16). The method then replaces each data point with a computed data point that fits the localized polynomial. The derivative is then obtained by computing the derivative of each localized polynomial at each data point.

The standard normal variate (SNV) method is the second method of baseline correction. SNV performs a baseline correction by taking each value in the spectrum, subtracting the mean, and then dividing by the standard deviation of entire spectrum (3).

4.2. Developing Predictive Models

It was determined that the NIR was suitable to perform two important interrelated functions, each requiring the development of different predictive models. Function one is to determine the fuel type of an unknown sample, either diesel, JP-8, Jet-A, JP-5, or other. Function two is to determine the sample's specification rating, whether it is On-spec, Off-spec, and Out-of-spec, by determining the physical property of the sample. At the time of writing this paper 254 diesel samples, 63 JP-8 samples, and 4 jet-A samples had been obtained and evaluated. Due to the limited number of samples and data only models for determining fuel type and select diesel fuel properties could be constructed.

4.3. Soft Independent Modeling of Class Analogies Method (SIMCA)

The first function of the NIR spectrometer is determining fuel type using a soft independent modeling of class analogies method (SIMCA). SIMCA uses Principle Component Analysis (PCA) to model the shape and position of the samples in multidimensional space, by identifying important parts of the spectrum and eliminating noise (3). A principle component is a variable that incorporates the most variation possible in a dataset and is unrelated to the previous principle component of the same dataset.

Fuel samples were classified as to the fuel class that each fuel was sold as, being JP-8 or diesel. An acceptance region is then created in multidimensional space for each different type of fuel class. A problem was discovered in which there is the potential of crossover fuels between classes. A single fuel can be produced by a manufacturer and sold as Diesel No 1, and a jet fuel. The sample set used for building the model did not include any such overlapping data, but real

world data could wrongly classify these samples. Upon verification of this model 100 diesel samples were identified correctly, no independent JP-8 samples were tested.

The 3-D plot shown in Figure 1 shows a separation between the two fuel types with JP-8 fuels shown in red and diesel samples shown in blue. Evaluation of the 3-D plot clearly shows how samples could easily overlap from one fuel type to another. This can be logically understood with the knowledge that these two types of fuel are chemical mixtures that are very closely related to one another, and realistically contain many identical components. The addition of additional fuel types such as Jet-A, and JP-5 will hopefully aid in further separating the fuel classifications set up utilizing SIMCA.
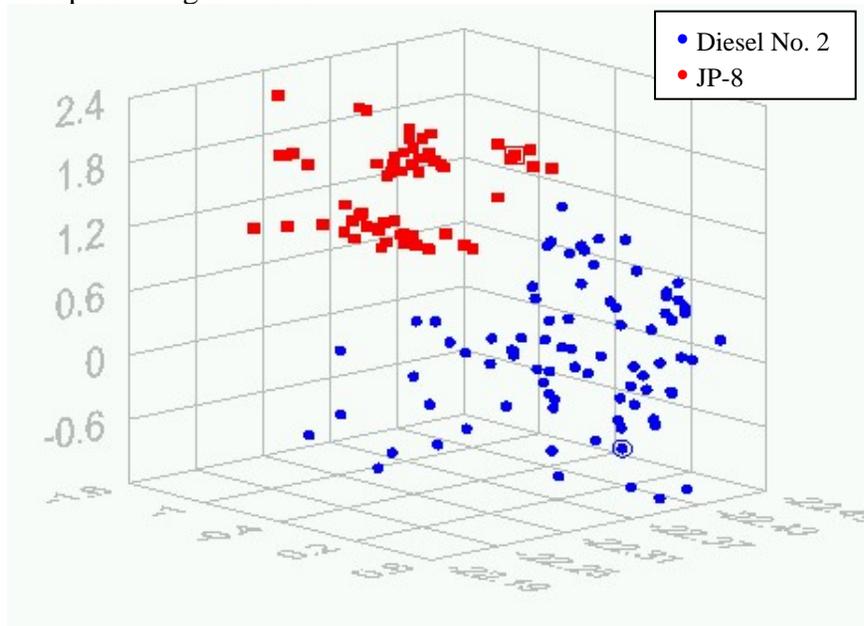
Figure 1 3D plot of SIMCA model evaluation

4.4. Partial Least Squares (PLS)

The next function of the NIR is to provide a prediction of the physical properties of the fuel, utilizing Partial Least Squares (PLS). PLS works by simplifying the sample spectrum into a small number principle components that are linear combinations of spectral absorption and wavelength. A least squares fit of the sample factors and the known physical property is then produced utilizing linear regression techniques (13). The correct number of sample principle components is essential to the establishment of PLS models, to few components will not accurately model the system, while too many components will create the modeling of noise from the calibration set. The result of PLS is a model that can be employed to predict the physical property of the fuel sample.

The available fuel samples were divided into a calibration set of 150 samples and a validation set of 100 samples. Diesel fuel physical property models have been successfully written for API gravity, boiling point at 50% and 90% distilled, cetane index, and cloud point. A flashpoint model was attempted but to marginal results.

4.4.1. API Gravity

The verification set for the API gravity model has a squared correlation coefficient (R^2) of .9329, and a standard error of prediction (SEP) of 0.83. The good correlation seen in this property is reasonable due to density being so closely related to the chemical composition of the fuel. The data for these samples was obtained utilizing ASTM D 1298, Standard Test Method for Density, Relative Density (Specific Gravity), or API Gravity of Crude Petroleum and Liquid Petroleum Products by Hydrometer Method, which has a published repeatability of 0.1 and reproducibility of 0.3 (17). The high repeatability and reproducibility of this method aids in the production of this model.
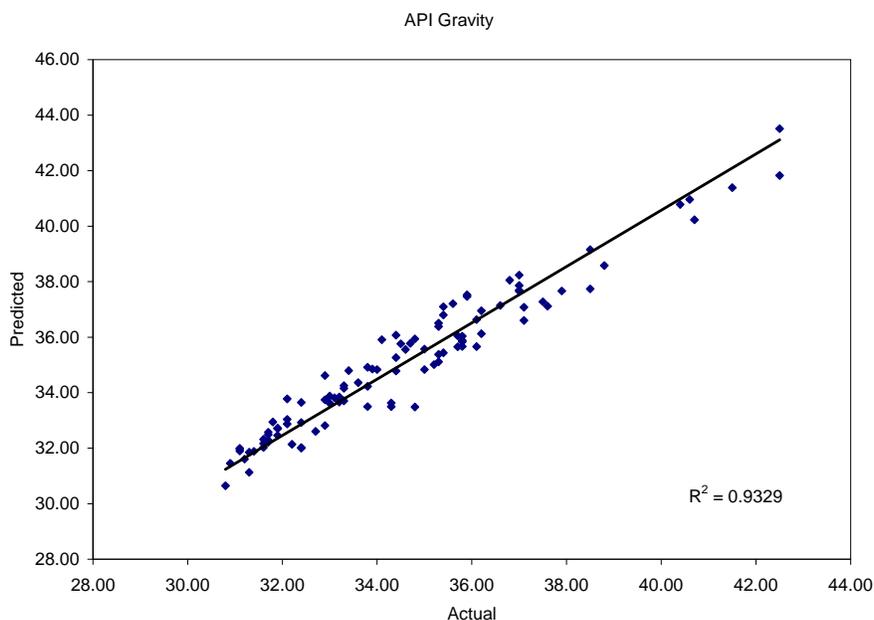
Figure 2 API gravity prediction by PLS

4.4.2. Cetane Index

The verification set for the cetane index model has a R^2 of .9418 and a SEP of 0.81 of a cetane number. The cetane index is calculated via data from API gravity and boiling point at 50% distilled, utilizing ASTM D 976 Standard Test Methods for Calculated Cetane Index of Distillate Fuels. The published error for this method is "somewhat less than +/-2 cetane numbers for 75 % of the distillate fuels evaluated" for fuels with a cetane number between 30 and 60 (18). The high correlation of this property is expected due to cetane being closely correlated to the chemical composition of the fuel as described in the "Introduction to Chemometrics and use in Near Infrared Spectroscopy" section earlier in this text.
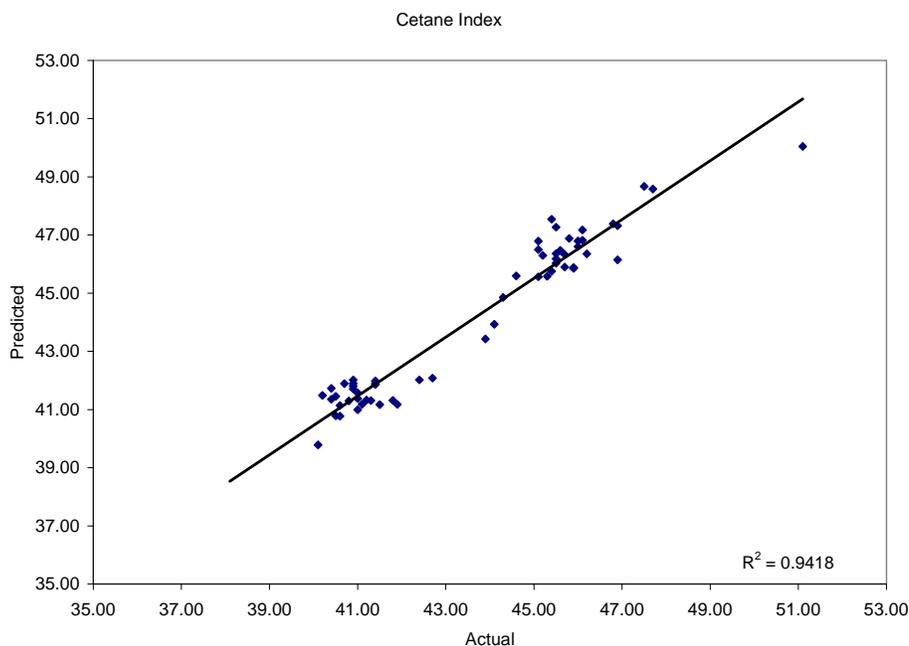
Cetane Index

Figure 3 Cetane Index prediction by PLS

4.4.3. Boiling point at 50% and 90% Distilled

The verification set for boiling point at 50% distilled has a R^2 of .7911, and a SEP of 4.90 ℃, while the verification set for boiling point at 90% distilled is .6719 and 7.70 ℃ respectively. The distillation boiling points are determined by ASTM D 86 Standard Test Method for Distillation of Petroleum Products at Atmospheric Pressure, which has a average repeatability and reproducibility of 1.8 ℃ and 4.6 ℃ at 50% distilled compared to a 2.52 ℃ and 4.93 ℃ respectively at 90% distilled (19). The relatively high variation that can be found within samples utilizing ASTM D 86 accounts for the error found in the PLS model, and decreased precision found in the model at 90% distilled can be attributed to the decrease in precision found in the reference technique.

Boiling Point at 50% Distilled

Figure 4 Boiling Point at 50% distilled prediction by PLS

Boiling Point at 90% Distilled
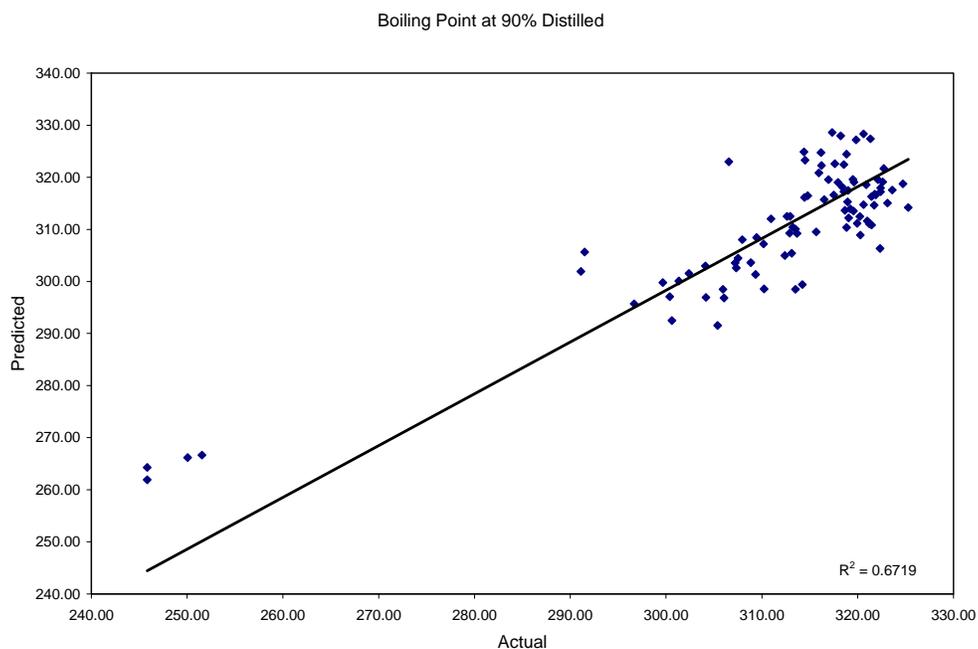
Figure 5 Boiling Point at 90% distilled prediction by PLS

4.4.4. Cloud Point

The cloud point verification set has a R^2 of .5377, and a SEP of 4.7 ºC. The cloud point is determined by ASTM D 2500 Standard Test Method for Cloud Point of Petroleum Products, which has a published repeatability of greater than 2 ºC in 1 case of 20 and reproducibility greater than 4 ºC in 1 case of 20 (20). The variation that can be found within samples utilizing

ASTM D 2500 can account for the error found in the PLS model, and validates this model as being acceptable.
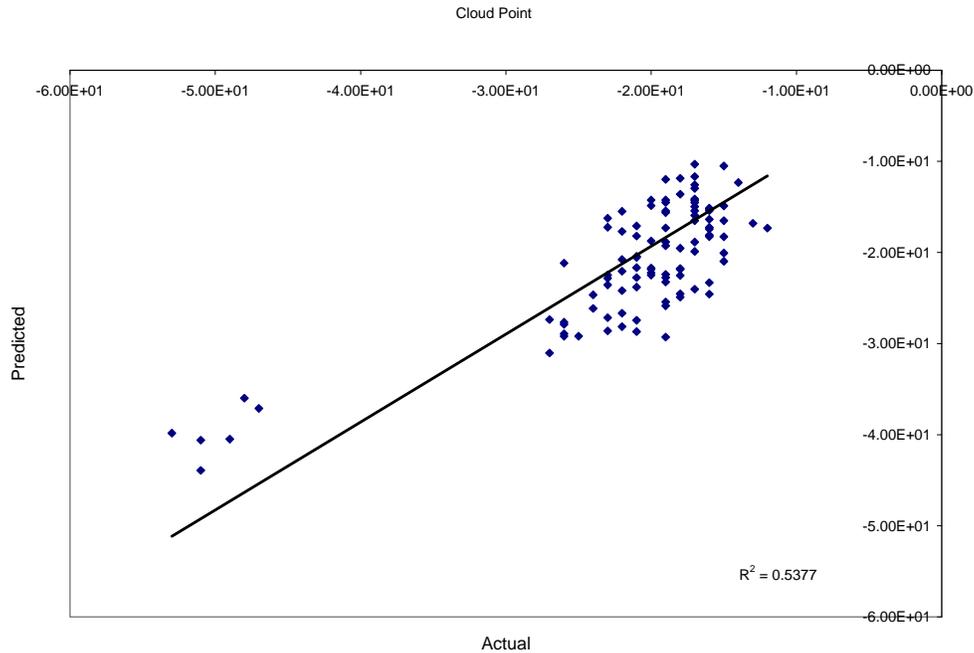
Cloud Point

Figure 6 Cloud Point prediction by PLS

4.4.5. Flashpoint

The verification set for flashpoint has a R^2 of -.8042, and a SEP of 3.38 degrees C. Flashpoint was determined utilizing a Pensky-Martens Closed Cup Tester according to ASTM D 93. The average repeatability of this test is 2.03 ºC with a reproducibility of 5.0 ºC (19). The relatively high variation that can be found within samples utilizing ASTM D 93 can account for the error found in the PLS model, but the correlation found in this model makes it so that this model can not be accepted. There appears to be a poor correlation appears between the predicted and known values for flashpoint but in analyzing the actual data the furthest off the predicted value was less than 8 ºC. All predicted values were still within acceptable limits as specified on table a. Further analysis will be directed into this area utilizing out of specification fuels to determine if this model can be further improved.
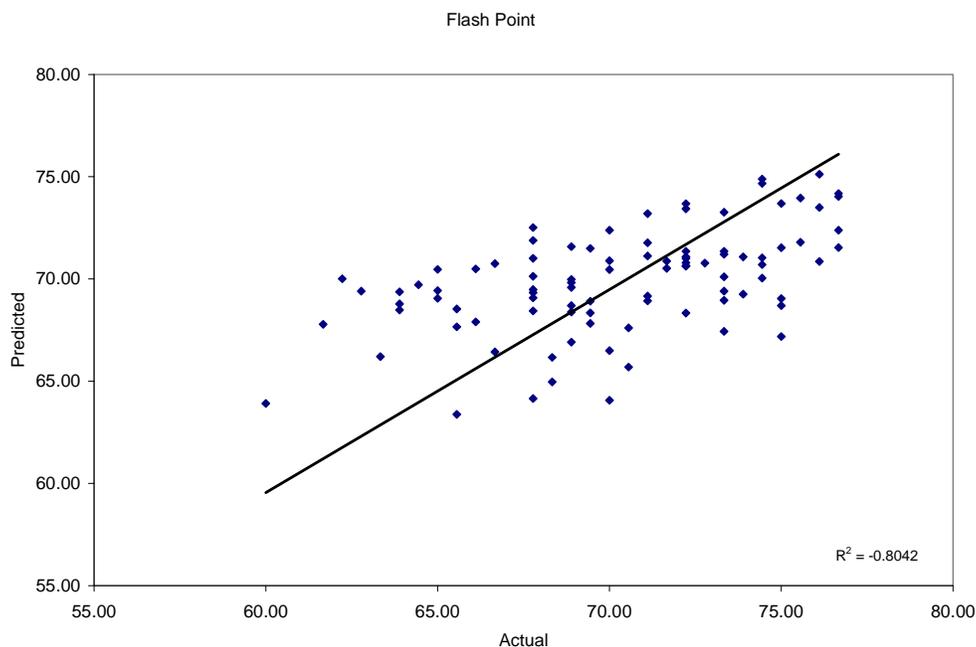
Flash Point

Figure 7 Flash Point prediction by PLS

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5. Conclusion

The application of NIR analysis has the shown the potential to provide rapid identification and analysis of fuels for selected properties as required to meet the requirements set forth for the Army's Petroleum Test Kit (PTK). Additional work is required to further define the desired models, and to produce models for the fuels that did not have adequate samples at the time of performing this preliminary study. ASTM data was based on single measurements, utilizing the accurate average of replicate data could significantly improve calibration models.

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Appendix A

Property	NIR test	B2 test	ASTM methods	ON SPEC	
				Low Sulfur #1 D	Low Sulfur #2 D
Water & Sediment % vol, max.		x	D2709, D1796	0.05	0.05
Distillation temp C 90% recovered, % vol.	x	x	D86	288 max	282 min; 338 max
Distillation temp C 50% recovered, % vol.	x		d86	Report	Report
Copper strip corrosion, rating max 3 hr @ 50C		x	D130	#3	#3
Flashpoint degree C min	x	x	D93	38	52
Kinematic viscosity, mm^2/S @ 40C		x	D445	1.3 min; 2.4 max	1.9 min; 4.1 max
Ash, % mass max			D482	0.01	0.01
Sulfur, % mass, max		x	D2622	0.05	0.05
Cetane number, min.			D613; D4737	40	40
Cetane index, min.	x	x	D976	40	40
Aromacity, % vol. max.	x		D1319	35	35
Cloud point, degree C max	x	x	D2500	note in spec D975	
Ramsbottom carbon residue on 10% distillation residue		x	D524	0.15	0.35
particulate contamination (gravimetric), mg/L		x	D6217	10	10
appearance		x	D4176	Report	Report
Saybolt color		x	D156	Report	Report
density/API gravity	x	x	D1298	Report	Report
pour point	x	x	D97	Report	Report

Table A-1. Tests and limits for diesel fuel

Property	OFF SPEC		OUT OF SPEC	
	Low Sulfur #1 D	Low Sulfur #2 D	Low Sulfur #1 D	Low Sulfur #2 D
Water & Sediment % vol, max.	>0.05	>0.05	>0.05	>0.05
Distillation temp C 90% recovered, % vol.	293	277 min; 343 max	>343	>343
Distillation temp C 50% recovered, % vol.	Report	Report	Report	Report
Copper strip corrosion, rating max 3 hr @ 50C	not #3	not #3	not #3	not #3
Flashpoint degree C min	<38	<52	<38	<52
Kinematic viscosity, mm^2/S @ 40C	Report	Report	Report	Report
Ash, % mass max	>0.01	>0.01	>0.01	>0.01
Sulfur, % mass, max	>0.05	>0.05	>0.05	>0.05
Cetane number, min.	>40	>40	>40	>40
Cetane index, min.	>40	>40	>40	>40
Aromacity, % vol. max.	>35	>35	>35	>35
Cloud point, degree C max				
Ramsbottom carbon residue on 10% distillation residue	>0.15	>0.35	>0.15	>0.35
particulate contamination (gravimetric), mg/L	20	20	greater than 20	greater than 20
appearance	haze/particulates	haze/particulates	haze/particulates	haze/particulates
Saybolt color	Report	Report	Report	Report
density/API gravity	Report	Report	Report	Report
pour point	Report	Report	Report	Report

Table A-2. Tests and limits for diesel fuel (continued)

Property	NIR Test	B2 Test	ASTM methods	ON SPEC
appearance		x		report
color (visual)		x		report
density (API)*	x	x	D1298, 4052	0.775-0.840
particulate matter (mg/L)		x	D2276, 5424	1
distillation*	x	x	D86, 2887	***
10% recovered			***	10 % recovered at 205 C
end point			***	300 C
residue, vol %			***	1.5
loss, vol %			***	1.5
copper strip corrosion (2 hr @ 100C/212F		x	D130	No. 1
freezing point (degrees C)* max	x	x	D2386, 5901, 5972	-47
existent gum, mg/100 ml		x	D381	7 mg/100 ml
flashpoint*	x	x	D56, 93, 3828	<38 C
water reaction		x	D1094	1 b
lead content (if cont with leaded fuel)		x	D323	NA
FSII (% vol)	x	x	D5006	0.10-0.15
filtration time (minutes)		x	App A MIL-DTL-83133	15
WSIM (MSEP rating)*		x	D3948	****
AO, MDA			***	90
AO, MDA, FSII			***	85
AO, MDA, CI/LI			***	80
AO, MDA, FSII and CI/LI			***	70
conductivity (pS/m)		x	D2624	150 and 450
thermal stability		x	D3241	***
change in pressure drop, mm Hg			***	25
heater tube deposit, visual rating			***	<3
Saybolt color		x	D156, 6045	to be reported
acid number		x	D3242	0.015 mg KOH/gm
aromatics (vol %)	x		D1319	25
viscosity, mm2/S @ 40C, max.	x		D445	8
net heat of combustion	x		D4809	42.8 mJ/kg (18400 BTU/lb)
hydrogen content, mass %	x		D3701	13.4

Table A-3. Tests and limits for JP-8 fuel

Property	OFF SPEC	OUT OF SPEC
appearance	Report	Report
color (visual)	Report	Report
density (API)*	30.9-54 API	outside range 30.9-54API
particulate matter (mg/L)	2	Greater than 2.0
distillation*	***	***
10% recovered	7% recovered at 205 C	<7% recovered at 205 C
end point	not listed	not listed
residue, vol %	2	>2
loss, vol %	not listed	not listed
copper strip corrosion (2 hr @ 100C/212F	No. 1	
freezing point (degrees C)* max	<-47	<-47
existent gum, mg/100 ml	14	outside range 7-14
flashpoint*	<38	<38 C
water reaction	1 b	not listed
lead content (if cont with leaded fuel)	14	
FSII (% vol)	0.09-0.20	outside range 0.09-0.2
filtration time (minutes)	20	greater than 20 minutes
WSIM (MSEP rating)*	***	***
AO, MDA	<90	<90
AO, MDA, FSII	<85	<85
AO, MDA, CI/LI	<80	<80
AO, MDA, FSII and CI/LI	<70	<70
conductivity (pS/m)	50-700	outside range 50-700
thermal stability	***	***
change in pressure drop, mm Hg	Report	Report
heater tube deposit, visual rating	Report	Report
Saybolt color	to be reported	to be reported
acid number	<0.015 mg KOH/gm	<0.015 mg KOH/gm
aromatics (vol %)	6.2-25	outside range 10-25%
viscosity, mm2/S @ 40C, max.	<8	>8
net heat of combustion	Report	Report
hydrogen content, mass %	13.0-27	outside the range 13-27

Table A-4. Tests and limits for JP-8 fuel (continued)

property	NIR Test	B2 test	ASTM Methods
appearance		x	
color (visual)		x	
density (API)*	x	x	D1298, 4052
particulate matter (mg/L)		x	D2276, 5424
distillation*	x	x	D86, 2887
10% recovered			***
end point (final boiling point)			***
residue, vol %			***
loss, vol %			***
copper strip corrosion (2 hr @ 100C/212F		x	D130
freezing point (degrees C)*	x	x	D2386, 5901, 5972, D4305
existent gum, mg/L		x	D381
flashpoint*	x	x	D56, 3828
water reaction		x	D1094
lead content (if cont with leaded fuel)		x	D323
FSII (% vol)	x	x	D5006
filtration time (minutes)		x	App A MIL-DTL-83133
WSIM (MSEP rating)*		x	D3948
AO, MDA			***
AO, MDA, FSII			***
AO, MDA, CI/LI			***
AO, MDA, FSII and CI/LI			***
conductivity (pS/m)		x	D2624
thermal stability (JFTOT) 2.5 hr @ 260 C		x	D3241
change in pressure drop, mm Hg			***
heater tube deposit, visual rating			***
Saybolt color		x	D156, 6045
acid number		x	D3242
aromatics (vol %)	x		D1319
viscosity	x		D445
net heat of combustion	x		D4809, D4529, D3338
hydrogen content, mass %	x		D3701

Table A-5. Tests and limits for Jet-A fuel

property	ON SPEC	OFF SPEC	OUT OF SPEC
appearance	Report	Report	Report
color (visual)	Report	Report	Report
density (API)*	0.775-0.840		
particulate matter (mg/L)	1	2	Greater than 2.0
distillation*	***	***	***
10% recovered	10 % recovered at 205 C	7% recovered at 205 C	
end point (final boiling point)	300 C	not listed	not listed
residue, vol %	1.5	2	>2
loss, vol %	1.5	not listed	not listed
copper strip corrosion (2 hr @ 100C/212F	No. 1	No. 1	not #1
freezing point (degrees C)*	(-47)' A1'; -40 A	<-47	<-47
existent gum, mg/L	7 mg/100 ml	14	outside range 7-14
flashpoint*	<38 C	<38 C	<38 C
water reaction	1 b	1 b	not listed
lead content (if cont with leaded fuel)	NA	14	>14
FSII (% vol)	0.10-0.15	0.09-0.20	outside range 0.09-0.2
filtration time (minutes)	15	20	greater than 20 minutes
WSIM (MSEP rating)*	****	***	***
AO, MDA	90	<90	<90
AO, MDA, FSII	85	<85	<85
AO, MDA, CI/LI	80	<80	<80
AO, MDA, FSII and CI/LI	70	<70	<70
conductivity (pS/m)	50 and 450	50-700	outside range 50-700
thermal stability (JFTOT) 2.5 hr @ 260 C	***	***	***
change in pressure drop, mm Hg	25	Report	Report
heater tube deposit, visual rating	<3	Report	Report
Saybolt color	Report	Report	Report
acid number	0.10 mg KOH/gm	<0.015 mg KOH/gm	<0.015 mg KOH/gm
aromatics (vol %)	25	<25%	<25%
viscosity	8		
net heat of combustion	42.8 mJ/kg (18400 BTU/lb)		
hydrogen content, mass %	13.4	<13.4	<13.4

Table A-6. Tests and limits for Jet-A fuel (continued)

Property	NIR Test	B2 Test	ASTM Method	ON SPEC
appearance		x		Report
color (visual)		x		Report
Density at 15 C, kg/L, min (API max)	x	x	D1298, D4052	(0.788-0.845) 36-48
particulate matter (mg/L)		x	D5424	1
Distillation, degrees C	x	x	D86	***
10% recovered, temp			D86	206 C max (185 C)
end point, temp			D86	300 (330 C)
residue, vol % max for D86			D86	1.5
loss, vol%, max			D86	1.5
copper strip corrosion, 2 hr @100 C, max.		x	D130	No. 1
Freezing Point, Max. C	x	x	D5972	-46 (-51) C max
Existent Gum		x	D381	7 mg/100 ml
Flashpoint	x	x	D56, D6450 (auto)	60 (140) min
FSII, % vol	x	x	D5006	0.15-0.20
filtration time (minutes)		x	App A MIL-DTL-83133	15
WSIM		x	D 3948	***
AO, MDA			D 3948	90
AO, MDA, FSII			D 3948	85
AO, MDA, CI/LI			D 3948	80
AO, MDA, FSII and CI/LI			D 3948	70
Conductivity		x	D2624	NA
Saybolt color		x	D156, D6045	report
Total Acid number, mg KOH/g, max		x	D3242	0.015
Aromatics, vol%, max		x	D1319	25
OR Doctor test			D4952	negative
kinematic viscosity, at -20 C, max, mm2/s	x		D445	8.5 max.
Flashpoint, C	x	x	D56, D93, D3828	60 min.
Vapor pressure, at 37.8 C (100 F), kPa			D323, D4953, D5190, D5191	14-21
Net Heat of Combustion, MJ/kg	x		D3338 or D4809	min. 42.6 MJ/kg
hydrogen content, mass %	x		D3701	13.4

Table A-7. Tests and limits for JP-5 fuel

Property	OFF SPEC	OUT OF SPEC
appearance	Report	Report
color (visual)	Report	Report
Density at 15 C, kg/L, min (API max)	36-53 API	outside range 36-53 API
particulate matter (mg/L)	2	>2
Distillation, degrees C	***	***
10% recovered, temp	>206 C	>206 C
end point, temp	>300 C	>300C
residue, vol % max for D86	>1.5	>1.5
loss, vol%, max	>1.5	>1.5
copper strip corrosion, 2 hr @100 C, max.	No. 1	Not No. 1
Freezing Point, Max. C	NA	less than -47C
Existent Gum	14	>14
Flashpoint	54-60	less than 60
FSII, % vol	0.10-0.20	<0.1
filtration time (minutes)	20	greater than 20 minutes
WSIM	***	***
AO, MDA	<90	<90
AO, MDA, FSII	<85	<85
AO, MDA, CI/LI	<80	<80
AO, MDA, FSII and CI/LI	<70	<70
Conductivity	NA	NA
Saybolt color	report	report
Total Acid number, mg KOH/g, max	>0.015	>0.015
Aromatics, vol%, max	7.1-25	outside range 7.1-25
OR Doctor test	negative	positive
kinematic viscosity, at -20 C, max, mm2/s	max. 8.5	>8.5
Flashpoint, C	<60	<60
Vapor pressure, at 37.8 C (100 F), kPa	outside range 14-21	outside range 14-21
Net Heat of Combustion, MJ/kg	<42.6	<42.6
hydrogen content, mass %	13.2-16.2	outside the range 13.2-16.2

Table A-8. Tests and limits for JP-5 fuel (continued)